IN THE CLAIMS:

1. (Currently amended) A computer-implemented method for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, wherein the method is run on a system comprising one or more distinct devices, each of the one or more distinct devices being embodied on a tangible computer-readable recordable storage medium, the method comprising:

calculating a centroid of residue centroids, wherein calculating the centroid of residue centroids is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of calculating the centroid;

using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment, wherein using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the centroid as a spatial origin;

calculating a first-order hydrophobic moment, wherein calculating the first-order hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of calculating the first-order hydrophobic moment;

enhancing correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric, wherein enhancing correlation between residue centroid magnitude and residue solvent accessibility is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of enhancing correlation;

using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment comprises measuring a fractional distance of each residue centroid to an

ellipsoidal surface of the tertiary protein structure, and mapping each ellipsoidal coordinate onto a sphere with radius equal to a major principal axis if a residue centroid has a same fractional distance from a center of the protein structure to the ellipsoidal surface of the tertiary protein structure as one or more additional residue centroids, wherein mapping places each residue at a same distance from the center of the protein structure to enable that each such residue that has the same fractional distance from the center of the protein structure contributes an equivalent magnitude to the global linear hydrophobic moment, wherein the global linear hydrophobic moment is calculated as $\vec{h}_1 = \frac{1}{n}\sum_i h_i(x_i\hat{i} + \sqrt{g'_2}\, y_i\hat{j} + \sqrt{g'_3}\, z_i\hat{k})$, wherein $\vec{h}_1$ comprises the first-order hydrophobic moment given by the global linear hydrophobic moment, n comprises a total number of residues, h_i comprises an origin of distribution, wherein the origin of distribution is the residue centroids, x_i, y_i and z_i comprise coordinates having the centroid of the residue centroids as the origin, $\hat{i}$, $\hat{j}$, *and* $\hat{k}$ comprise unit vectors along directions of principle axes used in the mapping of each ellipsoidal coordinate onto a sphere with radius equal to a principal axis, and g'_2 and g'_3 comprise scaled moments-of-geometry used to provide an ellipsoidal characterization of the protein structure via $g_1x_p^2 + g_2y_p^2 + g_3z_p^2 = d^2$, wherein g_1, g_2 and g_3 are moments-of-geometry, x_p, y_p and z_p are coordinates in a frame of the principle axes with the centroid of the protein structure as origin and d is a distance measure, further wherein $x_{ip}^2 + g'_2\, y_{ip}^2 + g'_3\, z_{ip}^2 = d'^2_i$, with $g'_2 = g_2/g_1$; $g'_3 = g_2/g_1$; $d'^2 = d_i^2/g_1$, wherein d'_i is a measure of radial fractional distance of the *i*th residue from the center of the protein to the protein surface, and wherein using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment;

using the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure, wherein using the global linear hydrophobic moment to characterize the amphiphilicity of the tertiary protein structure is carried out by a tertiary protein structure analyzer executing on a computer configured to carry out the step of using the global linear hydrophobic moment to characterize the amphiphilicity of the tertiary protein structure; and

outputting the global linear hydrophobic moment to a user.

2. (Canceled)

3. (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

4. (Original) The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

5. (Original) The method of claim 1, wherein the centroid of residue centroids represents a geometric center of the tertiary protein structure.

6. (Cancelled)

7. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a magnitude of amphiphilicity of the tertiary protein structure.

8. (Original) The method of claim 1, wherein the global linear hydrophobic moment characterizes a direction of amphiphilicity of the tertiary protein structure.

9. (Original) The method of claim 1, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

10. (Cancelled)

11. (Cancelled)

12. (Cancelled)

13. (Cancelled)

14. (Currently amended) An apparatus for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, the apparatus comprising:

a memory; and

at least one processor operative to:

calculate a centroid of residue centroids;

use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

calculate a first-order hydrophobic moment;

enhance correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

use the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment comprises measuring a fractional distance of each residue centroid to an ellipsoidal surface of the tertiary protein structure, and mapping each ellipsoidal coordinate onto a sphere with radius equal to a major principal axis if a residue centroid has a same fractional distance from a center of the protein structure to the ellipsoidal

surface of the tertiary protein structure as one or more additional residue centroids, wherein mapping places each residue at a same distance from the center of the protein structure to enable that each such residue that has the same fractional distance from the center of the protein structure contributes an equivalent magnitude to the global linear hydrophobic moment, wherein the global linear hydrophobic moment is calculated as $\vec{h}_1 = \frac{1}{n}\sum_i h_i(x_i\hat{i} + \sqrt{g'_2}\,y_i\hat{j} + \sqrt{g'_3}\,z_i\hat{k})$, wherein $\vec{h}_1$ comprises the first-order hydrophobic moment given by the global linear hydrophobic moment, n comprises a total number of residues, h_i comprises an origin of distribution, wherein the origin of distribution is the residue centroids, x_i, y_i and z_i comprise coordinates having the centroid of the residue centroids as the origin, $\hat{i}$, $\hat{j}$, *and* $\hat{k}$ comprise unit vectors along directions of principle axes used in the mapping of each ellipsoidal coordinate onto a sphere with radius equal to a principal axis, and g'_2 and g'_3 comprise scaled moments-of-geometry used to provide an ellipsoidal characterization of the protein structure via $g_1x_p^2 + g_2y_p^2 + g_3z_p^2 = d^2$, wherein g_1, g_2 and g_3 are moments-of-geometry, x_p, y_p and z_p are coordinates in a frame of the principle axes with the centroid of the protein structure as origin and d is a distance measure, further wherein $x_{ip}^2 + g'_2\,y_{ip}^2 + g'_3\,z_{ip}^2 = d'^2_i$, with $g'_2 = g_2/g_1$; $g'_3 = g_2/g_1$; $d'^2 = d_i^2/g_1$, wherein d'_i is a measure of radial fractional distance of the ith residue from the center of the protein to the protein surface;

use the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

output the global linear hydrophobic moment to a user.

15. (Original) The apparatus of claim 14, wherein the centroid of the residue centroids represents a geometric center of the tertiary protein structure.

16. (Cancelled)

17. (Original) The apparatus of claim 14, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

18. (Canceled)

19. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

20. (Original) The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

21. (Currently amended) An article of manufacture for calculating a global hydrophobic moment of a tertiary protein structure comprising a plurality of residues, comprising:

a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a step for calculating a centroid of residue centroids;

a step for using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

a step for calculating a first-order hydrophobic moment;

a step for enhancing correlation between residue centroid magnitude and residue solvent accessibility, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric;

a step for using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, and wherein using the first-order hydrophobic moment and the enhanced correlation between residue centroid magnitude and residue solvent accessibility to calculate the global linear

hydrophobic moment comprises measuring a fractional distance of each residue centroid to an ellipsoidal surface of the tertiary protein structure, and mapping each ellipsoidal coordinate onto a sphere with radius equal to a major principal axis if a residue centroid has a same fractional distance from a center of the protein structure to the ellipsoidal surface of the tertiary protein structure as one or more additional residue centroids, wherein mapping places each residue at a same distance from the center of the protein structure to enable that each such residue that has the same fractional distance from the center of the protein structure contributes an equivalent magnitude to the global linear hydrophobic moment, wherein the global linear hydrophobic moment is calculated as $\vec{h}_1 = \frac{1}{n}\sum_i h_i(x_i\hat{i} + \sqrt{g'_2}\, y_i\hat{j} + \sqrt{g'_3}\, z_i\hat{k})$, wherein $\vec{h}_1$ comprises the first-order hydrophobic moment given by the global linear hydrophobic moment, n comprises a total number of residues, h_i comprises an origin of distribution, wherein the origin of distribution is the residue centroids, x_i, y_i and z_i comprise coordinates having the centroid of the residue centroids as the origin, $\hat{i}$, $\hat{j}$, *and* $\hat{k}$ comprise unit vectors along directions of principle axes used in the mapping of each ellipsoidal coordinate onto a sphere with radius equal to a principal axis, and g'_2 and g'_3 comprise scaled moments-of-geometry used to provide an ellipsoidal characterization of the protein structure via $g_1x_p^2 + g_2y_p^2 + g_3z_p^2 = d^2$, wherein g_1, g_2 and g_3 are moments-of-geometry, x_p, y_p and z_p are coordinates in a frame of the principle axes with the centroid of the protein structure as origin and d is a distance measure, further wherein $x_{ip}^2 + g'_2\, y_{ip}^2 + g'_3\, z_{ip}^2 = d'^2_i$, with $g'_2 = g_2/g_1$; $g'_3 = g_2/g_1$; $d'^2 = d_i^2/g_1$, wherein d'_i is a measure of radial fractional distance of the ith residue from the center of the protein to the protein surface;

a step for using the global linear hydrophobic moment to characterize an amphiphilicity of a tertiary protein structure; and

a step for outputting the global linear hydrophobic moment to a user.